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NUFT USNT Thermal Input Parameters

K.H. Lee

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This document describes the thermal input parameters required to run the USNT module of the NUFT code. The USNT module handles multi-component transport of multiple fluid phases and heat through porous and fractured media. The thermal input parameters required to model the heat transport by conduction, convection, and radiation are summarized, and the relevant mixing rules outlined. This is followed by a table that describes the thermal input parameters in a typical NUFT input file used for YMP thermal-hydrological calculations.

Most of the material presented here is summarized from the user's manual of the USNT module of NUFT (Nitao, 2000).

Thermal Conductivity

The code requires the effective bulk thermal conductivity of materials to compute the transport of heat by conduction. The thermal conductivity is a constitutive coefficient that must be measured experimentally as a function of fluid phase saturation. The user must input the bulk thermal conductivity, in the *rocktab* input block, at full saturation for each of the fluid phases in the model. For typical Yucca Mountain calculations, a liquid phase and a gas phase are present. If the thermal conductivity varies significantly with temperature over the range of temperatures modeled, then the temperature-dependence can also be supplied as part of the input.

Two options are available for typical Yucca Mountain thermal hydrology (TH) problems, where the porous medium contains a maximum of two phases, liquid and gas (α = liquid, gas). In the first option the total bulk thermal conductivity is calculated using a linear weighting of fluid phase saturation over NP phases

$$k^{bulk} = k^{dry} + \sum_{\alpha=1}^{NP} S_\alpha \left(k_\alpha^{sat} - k^{dry}\right)$$

where S_α is the saturation of fluid phase α, and the input parameters are

k^{dry} bulk thermal conductivity of the porous medium with no fluid in pores (W/m-C)

$k^{sat}{}_\alpha$ bulk thermal conductivity of the porous medium saturated by phase α (W/m-C).

This equation represents the most general form for specifying the bulk thermal conductivity, and applies to the case of a porous medium with multiple fluid phases as well as a porous medium with evacuated pores (no fluids). When there is at least one fluid in the pores, k^{bulk} is independent of the term k^{dry}. In typical Yucca Mountain TH calculations, with liquid and gas phases (α = l, g), the required input parameters are k^{dry}, $k^{sat}{}_l$, and $k^{sat}{}_g$, but k^{dry} is not used and therefore does not need to be specified accurately. However, NUFT still requires that some value of k^{dry} be specified.

The second option is a constant thermal conductivity independent of fluid-phase saturation. The user can also optionally use temperature dependent thermal conductivity with each of the two options given above. This is achieved by specifying a temperature dependent factor as a piecewise linear table. The thermal conductivity used in numerical calculations is obtained by multiplying the value from option one or two by the supplied factor.

Specific Heat of Dry Solids

Solution of the energy balance equation also requires specific heat of the solids and fluids that comprise the bulk porous medium. The specific heat of dry solids (J/kg-C) is required in the *rocktab* block of the input file. This is the specific heat at constant pressure, c_p, and not the specific heat at constant volume, c_v.

Heat Content of Fluids

Parameters required to calculate the heat content of fluid components are specified in the *compprop* block of the input file, and the mixing method used to compute the heat content of the phase is specified in *phaseprop*. The specific enthalpy, H (J/kg), of each chemical component is calculated using one of five options.

1. Constant value
   Input a value of H for constant specific enthalpy (J/kg)
2. Calculate H from the formula
   $H = c_p * (T - T_{ref}) + Hv$
   Input c_p: specific heat at constant pressure (J/kg-C)
   T_{ref}: reference temperature (C)
   H_v: reference enthalpy (J/kg).
3. Calculate H from the formula
   $H = C_p * (T - Tref) + a(T - T_c)^b$
   Input c_p: specific heat at constant pressure (J/kg-C)
   T_{ref}: reference temperature (C)
   T_c: critical temperature (C)
   a: parameter
   b: parameter
4. By specifying this option, the code uses the partial enthalpy of water in a pure aqueous phase, calculated from the steam tables; can be used, as an approximation, for dilute solutions.
5. By specifying this option, the code uses the partial enthalpy water in a pure water vapor phase; can be used, as an approximation, for water vapor in ideal gas mixtures.

Specific enthalpy of the phase is specified in the *phaseprop* input block of the code using one of the two options.

1. Input a constant specific enthalpy H (J/kg)
2. Select linear mixing of γ component partial enthalpies, H^γ, in α phase
   $H_\alpha = \sum_\gamma X_\alpha^\gamma H_\alpha^\gamma$
   where X^γ is the mass fraction of the γ component in the α phase.

Solid and Fluid Density

The solid grain density (kg/m^3) of each material is required input in the *rocktab* input block. The molecular mass (g/mole) of each component is required in *compprop*.

Parameters specifying the partial mass density of each component must be supplied in *compprop.* The density ρ, is calculated from the following formula based on constant compressibility.

$$\rho = \rho_0 \exp[c(p - p_0)]$$

The input parameters are

ρ_0	reference density (kg/m3)
p_0	reference pressure (Pa)
c	compressibility (1/Pa)

The user also has the option to select the partial mass density of pure liquid water calculated from the steam table; this is an approximation for a water component in a dilute aqueous phase.

The user is offered four options for calculating the phase mass density from the partial mass density of each component

1. Calculate the density, ρ, based on linear volumetric mixing

   $$\frac{1}{\rho} = \sum_{\gamma} \frac{X^{\gamma}}{\rho^{\gamma}}$$

   where X^{γ} and ρ^{γ} are the mass fraction and partial mass density of the γ component, respectively.
2. Phase density of the gas phase based on the ideal gas law. If there is a component called water, a "Z-factor" is used to correct the water vapor density from steam tables.
3. Phase density of the gas phase based on the ideal gas law.
4. Density of pure liquid water phase; can be used as an approximation for a dilute aqueous phase.

Equilibrium Partitioning

The user must supply parameters that specify the equilibrium partitioning of components between fluid phases. A convenient reference phase must be chosen for each component, and the partitioning coefficient, K_{eq}, for that reference phase set to unity. All other coefficients are then defined with respect to the reference phase. K_{eq} for a component in phase α is equal to the mole fraction of the component in the α phase divided by the mole fraction of the component in the reference phase. The code accepts four options for specifying K_{eq} in thermal models:

1. Constant coefficient (mole/mole)
2. $Keq = (A + pg * B + C / pg) * \exp(-D / TKelv)$

   where A, B, C, and D are user-specified parameters, pg is the gas pressure, and Tkelv is the temperature in Kelvin. Parameters A, B, and D are optional and default to zero. This formulation assumes that the liquid phase is the reference phase.

3. Select coefficient for TCE in gas phase, *KeqTCESolute*. Assumes that the liquid phase is the reference phase.

4. Select coefficient for water vapor in the gas phase, *KeqWatVapor*. Assumes that the liquid phase is the reference phase.

Source Term

Source terms, given in the *srctab* block of the input file, specify a mass or heat generation rate in a cell or range of cells, through a table of source fluxes at specified times. Component fluxes may be specified (including the energy component) using compflux, or phase fluxes using phaseflux. For a heat source, heating power (W) is tabulated versus time. Whenever a mass flux is specified an enthalpy table must be supplied to give the heat content of the components. The table gives specific partial enthalpies (J/kg) of the component as a function of time. Linear interpolation is used to calculate enthalpy between time values.

Thermal Radiation

The energy balance equation in NUFT handles the transfer of heat between elements by thermal radiation. This option is applied to model radiative heat transfer across surfaces such as waste package to drift wall, waste package to waste package, and drift wall to drift wall. The radiation flux, q_r, between two surfaces, 1 and 2, is given by

$$q_r = A_1 C \left[T_1^4 - T_2^4\right]$$

where A_1 is the surface area of face 1, C is a user-specified coefficient, and T_1 and T_2 are the absolute temperatures of surface 1 and surface 2, respectively. The user is expected to calculate C from

$$C = F\varepsilon\sigma,$$

where F is a view factor that depends on the geometry of the system, ε is the emissivity, and σ is the Stefan-Boltzmann constant. Any pair of surfaces across which radiative heat transfer is to be modeled, must have A_1 and C specified in the input file. For large numbers of radiation connections, the preprocessor RADPRO may be used to help the user specify connections and calculate coefficients.

DKM and ECM Models

The Dual Permeability Model (DKM) and the Equivalent Continuum Model (ECM) are two models commonly used to mathematically represent fracture-matrix interaction in TH calculations for Yucca Mountain. Each of these two models requires separate material input parameters, including thermal parameters, for the matrix and fractures. For example, a DKM input file must include separate thermal conductivity parameters for the rock matrix and the fractures.

Examples of NUFT Thermal Input

The following table describes the thermal input parameters typically used for YMP thermal-hydrological (TH) calculations with the NUFT code. I took one of the main input files used in TH calculations for the Large Block Test (LBT), highlighted the thermal input parameters, and used the table to describe usage of the parameters in NUFT input. Note that material properties are given for several materials, but the thermal parameters for just one material needs to be highlighted and described here. The LBT input file, lbt_AMR_ds, is shown in Attachment 1. The file includes another file, vt-rmsew.pkg, which in turn, includes the file vtough.pkg. vtough.pkg has some thermal input parameters, and is therefore shown in Attachment 2. These included files specify numerical settings, chemical components, and phases for typical YMP TH problems. Thermal parameters and input options selected in vtough.pkg are also highlighted and addressed in the table. The NUFT thermal radiation option was not used in LBT calculations addressed here. However, an example of radiation input parameters is included in the table, since radiation is frequently used in our YMP TH calculations.

NUFT Thermal Input Parameters

Main Data Block	Input Format and Parameters	Description of Input
Modprop	(modprop (tcond (range "UT*") (0.0 1.0 1.08e7 1.0 (1.081e7 .527 1e30 .527))	*Modprop* is an optional command to modify the thermal conductivity for a range of cells, specified in rocktab, by a time-dependent factor. Linear interpolation used between times in table.
Rocktab	(rocktab (m-tsw34 (solid-density 2.505e+03)…	Grain density of solids for material m-tsw34 set to 2505 kg/m^3
Rocktab	(rocktab (m-tsw34 (Cp 9.480e+02)…	Specific heat for material m-tsw34 set to 948 J/kg-C
Rocktab	(rocktab (m-tsw34 (tcond tcondLin (solid 1.544) (liquid 2.307)(gas 1.544)…	Bulk thermal conductivity of m-tsw34 is 2.307 W/m-C saturated with liquid, and 1.544 W/m-C saturated with gas. Thermal conductivity at other saturations obtained by linear interpolation. The thermal conductivity value for solid is not used by the code when fluids are present, but is required in the input; can use any numerical value.
Srctab	(srctab (compflux (name heat1 (range "E1.m*") (table 0.0 111.98 15840 339.20)	Specification of a time-varying heat source from a specified range of elements (E1.m*). Heat output at different times is specified in table; linear interpolation used to obtain heat output at times between table values.

	(allocate-by-volume)...	*Allocate-by-volume* instructs NUFT to divide the total heat output from source elements in proportion to element volume. The compflux set *name*, heat1, is used for data output options.
Init-eqts	(init-eqts (thermal)...	Energy balance equation is solved when set to *thermal*; the energy balance equation is not solved when set to *isothermal.*
Phaseprop	(phaseprop (liquid (rhoP rhoPLiqWat)...	The *rhoP* option *rhoPLiqWat* selects the density of pure liquid water as the density of the aqueous phase; this is used as an approximation for a dilute aqueous phase.
Phaseprop	(phaseprop (liquid (enthP enthPLinearMix)...	The *enthP* option *enthPLinearMix* selects linear mixing of the component partial enthalpies to determine the aqueous phase enthalpy.
Phaseprop	(phaseprop (liquid (pcTemFac watPcTemFac)...	The *pcTemFac* keyword activates NUFT temperature-dependent capillary pressure. With the *watPcTemFac* option, the capillary pressure is multiplied by a temperature-dependent factor based on the capillary pressure of water.
Phaseprop	(phaseprop (gas (rhoP rhoPZFacStm)...	With the *rhoP* option *rhoPZFacStm*, phase density of the gas phase is based on the ideal gas law. If there is a component called *water*, a "Z-factor" is used from the steam tables to correct for the water vapor density.
Phaseprop	(phaseprop (gas (enthP enthPLinearMix)...	The *enthP* option *enthPLinearMix* selects linear mixing of the component partial enthalpies to determine the gas phase enthalpy.
Compprop	(compprop (water (intrinsic (MoleWt 18.0)) (gas (enthC enthCWatVap))...	The *enthC* option *enthCWatVap* selects the partial enthalpy of water in a pure water vapor phase; used as an approximation, for water vapor in ideal gas mixtures.
Compprop	(compprop (water (intrinsic (MoleWt 18.0)) (liquid (enthC enthCLiqWat))...	The *enthC* option *enthCLiqWat* selects the partial enthalpy of water component in a pure aqueous, calculated from steam tables; used as an approximation for dilute solutions.
Compprop	(compprop (water (intrinsic (MoleWt 18.0)) (liquid	The *rhoC* option *rhoCLiqWat* selects the partial mass density of a pure water phase, calculated from the steam tables; an approximation for water component in dilute

	(rhoC rhoCLiqWat))...	aqueous phase.
Compprop	(compprop (air (intrinsic (MoleWt 29.0)) (gas (enthC enthCConstCp (Cp 1009.0) (Tref 0.0) (Hv 0.0)))...	The *enthC* option *enthCConstCp* as used here calculates the specific enthalpy of component air from the formula $H = C_p * (T - Tref) + Hv$ where C_p is the specific heat (J/kg-C), Tref the reference temperature (C), and H_v the reference enthalpy (J/kg).
Compprop	(compprop (air (intrinsic (MoleWt 29.0)) (liquid (rhoC rhoCLiqWat))...	The *rhoC* option *rhoCLiqWat* gives a fictitious value for the partial mass density of air in the aqueous phase. This value is not used in PVT calculations because *rhoPZFacStm* does not use it; only used in chemical potential calculations.
Genmsh	(genmsh (radcon (add (Coef 2.37e-09) (A 1.0) (surface 4 4 5 5 4 4) (offset 3 -1 -2))...	The *radcon* data block within *genmsh* adds radiation connections between pairs of elements. Here the elements (4,5,4) and (7,4,2) are connected with a coefficient of 2.37e-09. See the NUFT USNT User's Manual for more details.

References

Nitao, J.J., User's manual for the USNT Module of the NUFT Code, Version 3.0, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MA-130653 Rev. 2., 2000.

Attachment 1: Example NUFT Input File

```
;; LBT AMR Calculations using basecase driftscale data
;; Running NUFT version: 3.0.1s (SUN/SOLARIS)
;; Assumes negligible thickness of boundary layer at outer insulator-
atm interface,
;;   so heat transfer to atm is controlled by conduction within the
Large Block and insulation
;;   and not by convection into atm (ie high Biot number); assume high
atm tcond of 2.60e03 W/m-C
;; System totally insulated by ultratemp, 0-125 days (0-1.0800e07 sec)
;; Virtually zero insulating effect of fiberglass prior to blow-in at
125 days
;; Ultratemp insulator tcond constant at 0.095 W/m-C for first 125
days, then, based on heat flux
;;   measurements in the block, equivalent tcond for the two insulators
combined adjusted to
;;   .05 W/m-C for 125d - 600d

;; 1D initialization imp-DKM, Active Fracture, Large Block Simulation
Run
;; Use initial liq sat of 0.75, based on neutron probe measurements
(Wilder et al, 1997)
;; Input file for 1-d initialization is lbt_AMR_ds-00_1d.in
;; Atmospheric temp and pressure fluctuations obtained from Site 8 data
for 1997
;; Average atm temp for 1997 was 16.3 C; monthly (average) fluctuations
incorporated into run

(usnt
  (title "LBT, imp-DKM,3D, Active Fractures, DS data, Sl_init 0.75")
  (modelname LBT_IMP_AFC)

  (rmsconv-norm rownorm)
  (rmstolerconv 1.0e-05)
  (include-pkg "vt-rmsew.pkg")

  (adaptive-ilu on)


  (tstop 600d)  ;; run for 125 days before insul increased (2-28 to 7-
3-97 with higher tcond)
  (time 0)
  (stepmax 1000000)
  (dtmax 1.728e+13)
  (dt .1)


(mult-cont-diff-harmonic off)
(tolerconv (P 1000.)(S 0.005)(X 0.005)(T 1.0))
(reltolerconv (P 0.005)(S 0.0)(X 0.0)(T 1.e-2))


;;
************************************************************************
*************************

;; System totally insulated by ultratemp, 0-125 days (0-1.0800e07 sec)
;; Virtually zero insulating effect of fiberglass prior to blow-in at
125 days
```

```
;; Ultratemp insulator tcond constant at 0.095 W/m-C for first 125
days, then, based on heat flux
;;   measurements in the block, equivalent tcond for the two insulators
combined adjusted to
;;   .05 W/m-C for 125d - 600d

      (modprop
             (tcond (range "FG*")(factor 0.0 1.0e6  1.0800e7 1.0e6
1.081e7 1.0  1e30 1.0))
             (tcond (range "UT*")(factor 0.0 1.0   1.0800e7 1.0
1.081e7 .527  1e30 .527))
      )   ;; fac of .527 for ultratemp insulator gives a tcond of .05
W/m-C


;;
************************************************************************
****************************

 (output

      (extool (continuum m)
              (file-ext ".m.ext")(range "*.m*")
            (variables S.liquid T P)
;;          (variables log10K0 S.liquid)

             (outtimes 0 100 1d 5d 10d 15d 20d 543.5h 575.5h 25d 30d
40d 42d 43d 46d 50d 55d 60d
                             64d 66d 70d 73d 75d 77d 80d 85d 90d 95d
100d  105d
                             110d 115d 120d 125d 127d 130d 133d
                            135d 140d 145d 150d 154.45d 160d 169d 175d
182.625d 192d
                            200d 222d 225d 230d 240d 250d 275d 279d 280d
282d 290d
                      300d 320d 340d 350d 365.25d 370d 375d 376d 377d
                      380d 385d 390d 400d 410d 425d 450d 475d 500d 550d
600d)
      )


      (extool (continuum f)
              (file-ext ".f.ext")(range "*.f*")
            (variables S.liquid T P)

             (outtimes 0 100 1d 5d 10d 15d 20d 543.5h 575.5h 25d 30d
40d 42d 43d 46d 50d 55d 60d
                             64d 66d 70d 73d 75d 77d 80d 85d 90d 95d
100d  105d
                             110d 115d 120d 125d 127d 130d 133d
                            135d 140d 145d 150d 154.45d 160d 169d 175d
182.625d 192d
                            200d 222d 225d 230d 240d 250d 275d 279d 280d
282d 290d
                      300d 320d 340d 350d 365.25d 370d 375d 376d 377d
                      380d 385d 390d 400d 410d 425d 450d 475d 500d 550d
600d)
```

```
      )


        (forcetimes
      (outtimes 2.592e06 1.080e7 1.081e7 3.241e7)
      )

;; write restart file at 30 days
      (restart
            (outtimes 30d)
            (file-ext  ".rst")
      )

;; output total heat flux lost through top of block at every timestep
     (flux-history
                (variable Q.energy)
                (crange
                        ("tsw34.m#*:*:3"  "tsw34.m#*:*:2")
                        ("tsw34.f#*:*:3"  "tsw34.f#*:*:2"))
                (outtimes *)
                (file-ext ".htflux_tot_top")
     )

;; output conductive heat flux through top of block at every timestep
     (flux-history
                (variable  Qcond)
                (crange
                        ("tsw34.m#*:*:3"  "tsw34.m#*:*:2")
                        ("tsw34.f#*:*:3"  "tsw34.f#*:*:2"))
                (outtimes *)
                (file-ext ".htflux_cond_top")
     )

;; output advective heat flux through top of block at every timestep
     (flux-history
                (variable  Qa.energy)
                (crange
                        ("tsw34.m#*:*:3"  "tsw34.m#*:*:2")
                        ("tsw34.f#*:*:3"  "tsw34.f#*:*:2"))
                (outtimes *)
                (file-ext ".htflux_advect_top")
     )



) ;; end output

;;
***********************************************************************
**************************

  (rocktab
;; imp-DKM-active-fracture version

(m-tsw34   ;; Driftscale data
  (cont-len-fac 3.858e-02) (cont-area-fac 1.354e+01)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
  (solid-density 2.505e+03) (porosity 1.100e-01)
  (Kd        (water 0.0) (air 0.0))
  (KdFactor  (water 0.0) (air 0.0))
  (Cp 9.480e+02)
  (tcond tcondLin (solid 1.544e+00) (liquid 2.307e+00) (gas 1.544e+00))
  (K0 4.070e-18) (K1 4.070e-18) (K2 4.070e-18)
  (tort (gas 7.000e-01) (liquid 0.000e+00))
  (kr (liquid krlVanGen (Sr 1.900e-01) (m 2.910e-01) (Smax 1.0))
      (gas krgModCorey (Srl 1.900e-01) (m 2.910e-01) (Slmax 1.0)))
  (pc (liquid pcVanGen (Sr 1.900e-01) (m 2.910e-01) (alpha 3.860e-06)
(Smax 1.0)))
  (krMC (liquid  krMCintrinsic) (gas  krMCintrinsic))
) ;;End of the material

(f-tsw34    ;; Driftscale data
  (cont-len-fac 1.157e-03) (cont-area-fac 1.000e+00)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
  (solid-density 2.530e+01) (porosity 1.000e-02)
  (Kd        (water 0.0) (air 0.0))
  (KdFactor  (water 0.0) (air 0.0))
  (Cp 9.480e+02)
  (tcond tcondLin (solid 1.560e-02) (liquid 2.330e-02) (gas 1.560e-02))
  (K0 2.760e-13) (K1 2.760e-13) (K2 2.760e-13)
  (tort (gas 7.000e-01) (liquid 0.000e+00))
  (kr (liquid krlVanGen (Sr 1.000e-02) (m 6.080e-01) (Smax 1.0) (gamma
4.100e-01))
      (gas krgModCorey (Srl 1.000e-02) (m 6.080e-01) (Slmax 1.0)))
  (pc (liquid pcVanGen (Sr 1.000e-02) (m 6.080e-01)(alpha 5.160e-04)
(Smax 1.0) (gamma 4.100e-01)))
  (krMC (liquid  krMCactiveFrac (gamma 4.100e-01) (Sr 1.000e-02))
        (gas     krMCactiveFrac (gamma 4.100e-01) (Sr 0.0)))
) ;;End of the material


   (m-fbgls
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e-01)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 0.01) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
;;      (Cp 7.00e+02) (solid-density 25.00)
      (Cp 7.00e+02) (solid-density 24.975)
;;        (tcond tcondLin (solid .042)(liquid .042)(gas .042)) ;; bulk
value from supplier
;;        (tcond tcondLin (solid .0174)(liquid .0174)(gas .0174)) ;;
adjusted for layer thickness
;;        (tcond tcondLin (solid .01738)(liquid .01738)(gas .01738)) ;;
Kthm=Kthb(1 - phif)
      (tcond tcondLin (solid .04995)(liquid .04995)(gas .04995)) ;;
from ht flux; Kthm=Kthb(1 - phif)
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 0.0)
          (liquid 1.0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCintrinsic) (gas  krMCintrinsic))
    )
    (f-fbgls
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e+000)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 1.0e-03) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 7.00e02) (solid-density .025)
;;      (tcond tcondLin (solid 1.74e-05)(liquid 1.74e-05)(gas 1.74e-
05)) ;; Kthf=Kthb(phif)
      (tcond tcondLin (solid 5.0e-05)(liquid 5.0e-05)(gas 5.0e-05)) ;;
from ht flux; Kthf=Kthb(phif)
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 0)
          (liquid 0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCactiveFrac (gamma 4.100e-01) (Sr 1.000e-02))
        (gas     krMCactiveFrac (gamma 4.100e-01) (Sr 0.0)))

    )

   (m-ultmp
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e-01)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 0.01) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
;;      (Cp 1130.0) (solid-density 560.00)  ;; rhob = 560
      (Cp 1130.0) (solid-density 559.440)    ;; rhom = rhob(1 - phif)
;;      (tcond tcondLin (solid .095)(liquid .095)(gas .095))    ;; bulk
Kth
      (tcond tcondLin (solid 0.0949)(gas 0.0949)(liquid 0.0949))  ;;
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 0.0)
          (liquid 0.0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCintrinsic) (gas  krMCintrinsic))
    )

    (f-ultmp
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e+000)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 1.0e-03) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
;;      (Cp 1130.0) (solid-density 560.00)
      (Cp 1130.0) (solid-density 0.5600)
      (tcond tcondLin (solid 9.5e-05)(liquid 9.5e-05)(gas 9.5e-05))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 0)
          (liquid 0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCactiveFrac (gamma 4.100e-01) (Sr 1.000e-02))
        (gas     krMCactiveFrac (gamma 4.100e-01) (Sr 0.0)))
    )


    (m-heatr
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e-01)
      (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 0.01) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.8886e+02) (solid-density 3.0812e+03)
      (tcond tcondLin (solid 14.420000)(liquid 14.42000)(gas
14.420000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCintrinsic) (gas  krMCintrinsic))
    )


    (f-heatr
      (cont-len-fac 1.000e-04) (cont-area-fac 1.000e+00)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 1.0e-04) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 3.850e+02) (solid-density .308)
      (tcond tcondLin (solid 0.0)(liquid 0.0)(gas 0.0))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
       (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
  (krMC (liquid  krMCactiveFrac (gamma 4.100e-01) (Sr 1.000e-02))
        (gas     krMCactiveFrac (gamma 4.100e-01) (Sr 0.0)))

    )


  (atm
      (cont-len-fac 4.900e-001) (cont-area-fac 2.040e+000)
  (exfac-adv (liquid 1.000e+00) (gas 1.000e+00))
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+03)
;;      (tcond tcondLin (solid .026)(liquid .026)(gas .026)) ;; .026 is
actual tcond for air
      (tcond tcondLin (solid 2.6e03)(liquid 2.6e03)(gas 2.6e03)) ;;air
tcond increased 10**5
      (K0 1.000e-08) (K1 1.000e-08) (K2 1.000e-08)
     ;;  (exfac-adv (liquid 1.000e+000) (gas 1.000e+000))
      (tort (gas 1.0) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
  (krMC (liquid  krMCintrinsic) (gas  krMCintrinsic))
```

```
     )

} ;; end rocktab


;;
*************************************************************************
**************************

  (srctab

   (compflux
       (comp energy)
       (name heat1)
;; total of 450 W per heater
       (range "E1.m*")
      (include "/data28/lbt_AMR_ms-00/lbt_heatr1_model.power")
             (allocate-by-volume)

     ) ;; end compflux


   (compflux
       (comp energy)
       (name heat2)
;; total of 450 W per heater
       (range "E2.m*")
      (include "/data28/lbt_AMR_ms-00/lbt_heatr2_model.power")

             (allocate-by-volume)

     ) ;; end compflux

   (compflux
       (comp energy)
       (name heat3)
;; total of 450 W per heater
       (range "E3.m*")
      (include "/data28/lbt_AMR_ms-00/lbt_heatr2_model.power")

             (allocate-by-volume)

     ) ;; end compflux


  ) ;; end srctab



     ;; set boundary conditions
     (bctab
;;    (surf
;;           (range  "at*")
;;           (basephase gas)
;;           (clamped)
;;    )
```

```
(topbc
            (range  "atl*")
            (basephase gas)
            (tables
                  (S.liquid  0.0 0.0  1.0e30 0.0)

                  (P         0.0 .886947e5  1.0e30 .886947e5)

                  (X.air
                        (include "/data28/lbt_AMR_ms-
00/lbt_topT_Xa.table")
                  )

                  (T
                        (include "/data28/lbt_AMR_ms-
00/lbt_topT_bc.table") ;; 0.80 RH at top bc
                  )
            )

)


      (atms   ;; side and floor
            (range  "att*")
            (basephase gas)
            (tables
                  (S.liquid  0.0 0.0  1.0e30 0.0)

                  (P         0.0 .886947e5  1.0e30 .886947e5)
            (X.air
                  (include "/data28/lbt_AMR_ms-00/LBT_xair_table"))

            (T
                  (include "/data28/lbt_AMR_ms-00/LBT_air_temp_table"))
            )
      )

      (bdry
            (range  "wt*")
            (clamped)
      )

      ) ;; end bctab



        ;; set initial conditions.

        (state
                (include "/data28/lbt_AMR_ds-00/lbt_AMR_ds-
00_1d.m.ztable")
                (include "/data28/lbt_AMR_ds-00/lbt_AMR_ds-
00_1d.f.ztable")

                (S.liquid by-key  ("E*" 0.0)("at*" 0.0)("FG*"
0.0)("UT*" 0.0)
            ("wt*" 1.0))
```

```
                (X.air by-key ("*" -1)("E*" 1.0)("at*" .9869604)("FG*"
1.0)("UT*" 1.0)
                              ("wt*" 1.0e-6))

        ) ;; end state


 (genmsh
;;    (anisotropic)
      (down 0. 0. 1.0)
      (coord rect)
      (multi-continua
;;          (type normal)
        (type rocktab)
        (continuum
         (name m)

      (dx  .04  .08  .15  .15  .14  .08  .14  .15  .12  .11  .08  ;;
1.24, heatr at nx = 1,6,11
             .10  .08  .08  .05  .10  .20  .3   .6   1.2  2.4  4.8  ;;
UT at 15, FG at 16
             9.6  19.2 .10e-30)    ;; nx = 25

      (dy  .12 .18  4*.20  .10 .10  .10 .10  .05  .10  .2 .4 .8 1.6 3.2
6.4 12.8 25.6 1.0e-30) ;; heatr: j=1,7
            ;; nj = 21
                                                        ;; insul:
j=11,12

      (dz  1.0e-30 .075 22*.12 .07  12*.12 .085 .09 .15 .15 3*.2 .3 .4
.55 1 2 4 8 16 32 53
           50     80     117.58
          1.0e-30) ;; nk = 58


;; heatr k=25, conc k=40, grvl k=41
                                                    ;; rck ends at
k=39


      (mat
            (at1   atm      1 nx     1  ny   1  1)
            (tsw34 m-tsw34    1 nx     1  ny   2  nz)
            (att2   atm      1 nx     1  ny  39 39)
            (att3   atm      17 17     1  ny   2  39)
            (att3   atm      1 nx     13 13    2  39)
;;          (CT  m-conc      1 nx    1  ny   40 40)
;;          (GV  m-grvl      1 nx     1  ny   41 41)
            (UT  m-ultmp    15 15     1  11    2 39)
            (UT  m-ultmp     1 15     11 11    2 39)
            (FG  m-fbgls    16 16     1  12    2 39)
            (FG  m-fbgls     1 16     12 12    2 39)
            (tsw34 m-tsw34     1 14      1  10   2  nz)
              (tsw34 m-tsw34    1 nx      1  ny   55 57) ;; tsw34
              (wt  m-tsw34    1 nx      1 ny    nz nz) ;; wt layer

            (E1  m-heatr     1 1      1  7    25 25)
            (E2  m-heatr      6 6       1  7     25 25)
            (E3  m-heatr     11 11      1  7     25 25)
      )


;;    nullify some unneeded blocks
      (null-blocks
            (18 nx    1  ny    1 38)
            (1  17    14 ny    1 38)     ;; total 0f 11,856 null blocks
      )


   ) ;; end continuum



        (continuum
          (name f)
          (flow-area-density ("*.f*" 1.0))
          (LenFirst  ("*.f*" 1.0))     ;; half-width of matrix block
                                       ;; in the exp dkm model, modified
by cont-len-fac in rocktab.
          (Len  ("*.f*" 1.0))      ;; half-width of "fracture",
modified by cont-len-fac in rocktab.


      (dx  .04  .08  .15  .15  .14  .08  .14  .15  .12  .11  .08  ;;
1.24, heatr at nx = 1,6,11
             .10  .08  .08  .05  .10  .20  .3   .6   1.2  2.4  4.8  ;;
UT at 15, FG at 16
             9.6  19.2 .10e-30)    ;; nx = 25

      (dy  .12 .18  4*.20  .10 .10  .10 .10  .05  .10  .2 .4 .8 1.6 3.2
6.4 12.8 25.6 1.0e-30) ;; heatr: j=1,7
           ;; nj = 21

;; insul: j=11,12

      (dz  1.0e-30 .075 22*.12 .07  12*.12 .085 .09 .15 .15 3*.2 .3 .4
.55 1 2 4 8 16 32 53
          50      80      117.58
         1.0e-30) ;; nk = 58

;; heatr k=25, conc k=40, grvl k=41
                                                       ;; rck ends at
k=39


      (mat
            (at1   atm      1 nx      1  ny   1  1)
            (tsw34 f-tsw34   1 nx      1  ny   2  nz)
            (att2   atm      1 nx     1  ny  39 39)
            (att3   atm      17 17     1  ny   2  39)
            (att3   atm      1 nx     13 13    2  39)
;;          (CT  f-conc      1 nx    1  ny    40 40)
;;          (GV  f-grvl      1 nx     1  ny   41 41)
```

```
            (UT  f-ultmp    15 15     1  11     2 39)
            (UT  f-ultmp     1 15    11 11      2 39)
            (FG  f-fbgls    16 16    1  12      2 39)
            (FG  f-fbgls     1 16    12 12      2 39)
            (tsw34 f-tsw34     1 14      1  10    2  nz)
              (tsw34 f-tsw34    1 nx      1  ny    55 57) ;; tsw34
              (wt  f-tsw34    1 nx     1 ny     nz nz) ;; wt layer
            (E1  f-heatr     1 1      1  7     25 25)
            (E2  f-heatr     6 6      1  7     25 25)
            (E3  f-heatr    11 11     1  7     25 25)

      )

;;    nullify some unneeded blocks
      (null-blocks
            (18 nx   1  ny   1 38)
            (1  17   14 ny   1 38)    ;; total 0f 11,856 null blocks
      )


   ) ;; end continuum


      ) ;; end multi-continua
) ;; end genmsh

         (redblk-cuthill-mckee off)
         (linear-solver pcg)
         ;;(eisenstat-walker on)
         (pcg-parameters  (precond d4) (north 25) (toler 1.e-1)
                          (itermax 200))
         (ilu-degree 2)  ;; increase to 2 (from 0) if you get maximum
                         ;; solver iterations exceeded

);; end of model input
```

Attachment 2: Included Input File vtough.pkg

```
;; SCCS_ID   @(#)vtough.pkg   1.4 09/29/99   NUFT_INPUT_FILE

;;; NUFT package for 2phase (liquid-gas), 2 mass component (air-water),
;;; non-isothermal model that is consistent with vtough-like
;;; usage:  (include-pkg "vtough.pkg")

;; history for 2p2ct.pkg
;; 4-15-94 changed Cp to be in J/kg C instead of J/mole C in
;;         keeping with change in model from mole balance to mass
balance

;; history for vtough.pkg
;; 4-27-94 created from 2p2ct.pkg
;; 5-3-94  use binGasKinetic instead of binGasFuller for free
diffusivity
;; 12-2-94 use 0.1 for reltolerdt for pressure
;; 4-11-95 input by mass fraction on
;; 6-26-96 changed air equilibrium constant
;; 12-13-97 added (pbase-largest-Keq off) because of this new option

    ;; input concentrations by mass fraction
    (input-mass-fraction on)
    ;; absolute time step tolerance
    ;; VTOUGH uses 8e5 but use 2e4 for tighter tolerance
    (tolerdt (P 2.e4)(S 0.3)(X 0.3)(T 20.))
    ;; relative time step tolerance
    ;; VTOUGH uses value of P of 0.0
    (reltolerdt (P 0.1)(S 0.0)(X 0.0)(T 0.0))
    ;; absolute NR conv. tolerance
    (tolerconv (P 1000.)(S 0.005)(X 0.005)(T 0.1))
    ;; absolute NR conv. tolerance
    (reltolerconv (P 0.005)(S 0.0)(X 0.0)(T 1.e-3))

    ;; in keeping with vtough (??) we choose base phase as the first
    ;; phase that exists in the ordering of init-eqts; this option
    ;; off gives the same results as previous versions of vtough.pkg
    (pbase-largest-Keq off)

    ;; if on, dependent concentrations will be forced to be between 0.0
and 1.0
    (dep-conc-inline off)

    ;; weighting for nonadvective density
    ;; if off, then model uses proportional distance weighting
    (one-half-density-weighting on)
    ;; weighting for advective densities
    ;; if off, then model uses same as option for nonadvective
densities)
    (upstream-advective-density off)

    (diffusion-geo-mean on) ;; use geometric mean of S*phi
                          ;; for factor multiplying diffusion coef.
                            ;; and simple 0.5 weighted average for tau


     ;; no diffusion at connections which have zero permeability
     (nodiff-where-noperm on)

     ;; equation setup
     (init-eqts
          (components water air)
          (phases liquid gas)
          (primary-phase gas)
          (wetting-phase liquid)
          (thermal)
     )

     ;; phase properties
     (phaseprop
          (liquid
             (rhoP rhoPLiqWat)
             (viscosity visLiqWat)
             (enthP enthPLinearMix)
           (pcTemFac watPcTemFac)
          )
          (gas
             (rhoP rhoPZFacStm)
             (viscosity visGasAirWat)
             (enthP enthPLinearMix)
          )
      ) ;; end phaseprop

     ;; component properties
     (compprop
          (water
                (intrinsic (MoleWt 18.))
                (gas
                         (Keq KeqWatVapor)
                   (freeDiffusivity binGasKinetic (power 1.8)(D0 2.13e-
5))
                         (enthC enthCWatVap))
                (liquid (freeDiffusivity 1.e-9) (Keq 1.0)
                         (enthC enthCLiqWat)
                         (rhoC rhoCLiqWat))
           )
          (air
                (intrinsic (MoleWt 29.))
                (gas (Keq KeqStd (C 6.65e9)(D 0.0))
                   (freeDiffusivity binGasKinetic (power 1.8)(D0 2.13e-
5))
                         (enthC enthCConstCp (Cp 1009.0)(Tref 0.0) (Hv
0.0)) )
                (liquid (freeDiffusivity 1.e-9)   (Keq 1.0) (enthC 0.0)
               (rhoC rhoCLiqWat)) ;; fictitious value not used in
                                     ;; pvt calculations because
rhoPZFacStm
                                     ;; doesnt use it; only used when
                                     ;; matrix-basis-pot is set to on
                                     ;; in order to compute chemical
                                     ;; potential

           )

     );;end component properties
```

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